

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.83 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.47e-01

Confidence level: 5.57e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Meglumine</div> <div>Measured: 3.62</div> <div>Predicted: 2.83</div>	<div>Image not found</div> <div>D-Glucose</div> <div>Measured: 4.08</div> <div>Predicted: 2.66</div>	<div>Image not found</div> <div>Galactose</div> <div>Measured: 4.08</div> <div>Predicted: 2.66</div>
<div>Image not found</div> <div>alpha-d-glucopyranose</div> <div>Measured: 4.08</div> <div>Predicted: 2.66</div>	<div>Image not found</div> <div>D-Mannose</div> <div>Measured: 4.08</div> <div>Predicted: 2.66</div>	<div>Image not found</div> <div>Pantothenic acid</div> <div>Measured: 4.56</div> <div>Predicted: 2.37</div>